



Clinical Bioinformatics: Linking Pharmacogenomics with Informatics

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Received: December 24, 2017; **Published:** February 27, 2018

Abstract

Pharmacogenomics focuses on personalized medicine to identify for individuals differences in disease diagnosis, experience, and therapy response. Integration of bioinformatics in pharmacogenomics offers reduction in healthcare costs by improving our ability to quickly and reliably select effective therapy for a given patient while minimizing costs associated with ineffective treatment and avoidable adverse events.

Keywords: String; Abalone; InPrePPI; CFinder; MCODE

Introduction

With the advancements in the field of clinical chemistry, biochemistry and microscopy, personalized medicine is becoming more and more popular, linking health with genes. Thus by documenting and probing people's family health histories for a diseases, genetic source is identified for the successive progeny [1,2]. With the passage of time valuable genomic data escalated identifying sets of genes that are involved in a disease among people of different ages, backgrounds and cultures [3]. Personalized medicine is recommending the drug based on an individual genomics.it is often considered as custom made drug based on individual characteristics, essentials and preferences [4,5]. Because a disease onset, prog-

nosis and response to a drug varies from individual to individual [6]. Genomic information plays an important role in personalized medicine. DNA-based technologies such as SNP genotyping, haplotype mapping or gene sequencing helps in identifying disease vulnerability and risk in an individual at birth [7,8]. Besides mRNAs and microRNAs profiling, molecular interactions, modelling and simulation provides a more precise means to understand the underlying disease mechanism [9]. It also helps in disease diagnosis and based on patient's genetic makeup therapy is recommended [10,11].

Given below is a list of some bioinformatic tools and databases that is help full in pharmacogenomics table 1.

SMART	Provides functional information about the protein [12]
AutoDock	For the prediction of protein complexes interaction [13]
HADDOCK	Predicts modelling and interaction of molecular complexes [14]
BIND	Bio complexes molecular interaction database [15]
MOE	An integrated software for modelling, visualization and drug designing [16]
STRING	An extensive database on molecular interactions [17]
MIMO	Comparison tool for the biological pathways [18]
IntAct	Tools for molecular interaction data analysis [19]
Graemlin	Used for scalable multiple network alignment [20]
Path BLAST	Search molecular interactions [21]
CFinder	For finding and visualizing the nodes [22]
MINT	Database, on functional interactions of biological molecules [23]
Gene Quiz	To search for altered patterns in the given data [24]
ClustalW	Gene or protein sequences comparison tool [25]
Abalone	Molecular modelling simulations of biological molecules [26]
Ascalaph	Molecular modelling tool [27]
Discovery studio	Modelling and simulation tool [28]
Amber	Biomolecules molecular dynamics simulation tool [29]
FoldX	To estimate molecular stability of either single protein or complexes [30]
Potential Drug Target Database	Database of drug targets [31]
MEGA	Phylogenetic tree construction tool [32]

MOLPHY /PAML	Phylogenetic analysis tool based on maximum likelihood method [33,34]
JStree	Phylogenetic trees viewing and editing tool [35]
TreeView	Phylogenetic trees viewing tool [36]
Jalview	Alignment editor tool [37]
STITCH	Database about metabolic pathways and molecular [38]
SuperTarget	Database that contains drug-target relations [39]
SNPdetector	Tool for sensitive SNP detection [40]
SNPHunter	Tool for SNP screening, selection, and acquisition [41]
Survival GWAS_SV	Software to handle large scale genome-wide data [42]
TissGDB	Tissue-specific gene annotation database [43]
scRNASeqDB	Gene expression profiling database in humans based on RNA sequence[44]
Cancer cell metabolism gene database	Database of cancer cell metabolism genes [45]
Tumor suppressor gene database	Tumor suppressor genes database [46]
PAHKB	Pulmonary Arterial Hypertension Knowledge Base [47]
Virus Finder	Find viruses and their integration sites in host DNA [48]
CNV annotator	For copy number variation (CNV) determination in humans [49]
VarWalker	Analysis of putative cancer [50]
NGS Catalog	Next generation sequencing databases in humans [51]
GenRev	Tool for extraction of subnetwork [52]
glad	Tool for gene length bias detection [53]
InPrePPI	Tool for the prediction of protein-protein interactions (PPIs) [54]
SNPKS	To find the SNP size in vertebrate genomes [55]
PharmGKB	Tools to track associations between genes and drugs [56]
SIDER 2	Contains information on marketed medicines and their recorded adverse drug reactions [57]
Comparative Toxicogenomics Database	Contain data on biological interactions and its associations with diseases [58]
Genomics of Drug sensitivity in cancer database	Data on the relationship between tumour cell genomics and sensitivity to anti-cancer agents [59]

Table 1: List of bioinformatic tools and databases in pharmacogenomics.

Conclusion

Pharmacogenomics and bioinformatics, together paved the pathway for personalized medicine to be introduced as an effective therapy for individuals based on their genome. Pharmacogenomics provides information related to an individual's response to a drug based on their genetics. This information is valuable in designing novel drugs and vaccines. Though, both of these disciplines are still in infancy and currently facing hurdles but holds immense potential to revolutionize the coming era of medicine.

Bibliography

- Whirl-Carrillo M., et al. "Pharmacogenomics knowledge for personalized medicine". *Clinical Pharmacology and Therapeutics* 92.4 (2012): 414-417.
- Kalow W. "Pharmacogenetics and pharmacogenomics: origin, status, and the hope for personalized medicine". *The Pharmacogenomics Journal* 6.3 (2006): 162-165.
- Squassina A., et al. "Realities and expectations of pharmacogenomics and personalized medicine: impact of translating genetic knowledge into clinical practice". *Pharmacogenomics* 11.8 (2010): 1149-1167.
- Ginsburg GS and Willard HF. "Genomic and personalized medicine: foundations and applications". *Translational Research* 154.6 (2009): 277-287.
- Xie HG and Frueh FW. "Pharmacogenomics steps toward personalized medicine". *Personalized Medicine* 2.4 (2005): 325-337.
- Abrahams E., et al. "The Personalized Medicine Coalition". *American Journal of Pharmacogenomics* 5.6 (2005): 345-355.
- Sadée W and Dai Z. "Pharmacogenetics/genomics and personalized medicine". *Human Molecular Genetics* 14.2 (2005): R207-R214.
- Piquette-Miller M and Grant DM. "The art and science of personalized medicine". *Clinical Pharmacology and Therapeutics* 81.3 (2007): 311-315.
- Wei CY., et al. "Pharmacogenomics of adverse drug reactions: implementing personalized medicine". *Human Molecular Genetics* 21.R1 (2012): R58-R65.
- Fernald GH., et al. "Bioinformatics challenges for personalized medicine". *Bioinformatics* 27.13 (2011): 1741-1748.
- Kalow W., et al. "Pharmacogenomics". CRC Press (2001).
- Letunic I., et al. "SMART 7: recent updates to the protein domain annotation resource". *Nucleic Acids Research* 40.D1 (2011): D302-D305.
- Morris GM., et al. "Using autodock for ligand-receptor docking". *Current Protocols in Bioinformatics* 8 (2008): 8-14.
- Dominguez C., et al. "HADDOCK: a protein-protein docking approach based on biochemical or biophysical information". *Journal of the American Chemical Society* 125.7 (2003): 1731-1737.
- Avila-Campillo I., et al. "BioNetBuilder: automatic integration of biological networks". *Bioinformatics* 23.3 (2006): 392-393.

16. Wang L., *et al.* "DEGseq: an R package for identifying differentially expressed genes from RNA-seq data". *Bioinformatics* 26.1 (2009): 136-138.
17. Jensen LJ., *et al.* "STRING 8-a global view on proteins and their functional interactions in 630 organisms". *Nucleic Acids Research* 37.1 (2008): D412-D416.
18. Aranda B., *et al.* "The IntAct molecular interaction database in 2010". *Nucleic Acids Research* 38.1 (2009): D525-D531.
19. Sharan R., *et al.* "Network-based prediction of protein function". *Molecular Systems Biology* 3.1 (2007): 88.
20. Vouzis PD and Sahinidis NV. "GPU-BLAST: using graphics processors to accelerate protein sequence alignment". *Bioinformatics* 27.2 (2010): 182-188.
21. Adamcsek B., *et al.* "CFinder: locating cliques and overlapping modules in biological networks". *Bioinformatics* 22.8 (2006): 1021-1023.
22. Zanzoni A., *et al.* "MINT: a Molecular INteraction database". *FEBS Letters* 513.1 (2002): 135-140.
23. Koski LB., *et al.* "AutoFACT: An Automatic Functional Annotation and Classification Tool". *BMC Bioinformatics* 6.1 (2005): 151.
24. Larkin MA., *et al.* "Clustal W and Clustal X version 2.0". *Bioinformatics* 23.21 (2007): 2947-2948.
25. Segall RS. "Comparing four-selected data mining software". In *Encyclopedia of Data Warehousing and Mining*, Second Edition. IGI Global (2009): 269-277.
26. Panda B and Krishnan NM. "Bioinformatics, systems biology, and systems medicine". *Genomic Medicine: Principles and Practice* 83 (2014).
27. Patel VV. "Correlation between cheminformatics and bioinformatics in drug discovery: a farsight of pharmacy-the millennium oath". *Journal of Drug Discovery and Therapeutics* 1.5 (2013): 95.
28. Rizvi SMD., *et al.* "A simple click by click protocol to perform docking: AutoDock 4.2 made easy for non-bioinformaticians". *EXCLI Journal* 12 (2013): 831-857.
29. Hartman AL., *et al.* "Introducing WATERS: a workflow for the alignment, taxonomy, and ecology of ribosomal sequences". *BMC Bioinformatics* 11.1 (2010): 317.
30. Van Durme J., *et al.* "A graphical interface for the FoldX force-field". *Bioinformatics* 27.12 (2011): 1711-1712.
31. Howard K. "The bioinformatics gold rush". *Scientific American* 283.1 (2000): 58-63.
32. Kumar S., *et al.* "MEGA: molecular evolutionary genetics analysis software for microcomputers". *Bioinformatics* 10.2 (1994): 189-191.
33. Fushiki D., *et al.* "Phylogenetic and bioinformatic analysis of gap junction-related proteins, innexins, pannexins and connexins". *Biomedical Research* 31.2 (2010): 133-142.
34. Yang Z. "PAML: a program package for phylogenetic analysis by maximum likelihood". *Bioinformatics* 13.5 (1995): 555-556.
35. Kumar V., *et al.* "Big Data Analytics: Bioinformatics Perspective". *International Journal of Innovations and Advancement in Computer Science* 5.6 (2016): 8-14.
36. Zhai Y., *et al.* "A web-based Tree View (TV) program for the visualization of phylogenetic trees". *Journal of Molecular Microbiology and Biotechnology* 4.1 (2002): 69-70.
37. Clamp M., *et al.* "The jalview java alignment editor". *Bioinformatics* 20.3 (2004): 426-427.
38. Siatkowski M., *et al.* "CellFateScout—a bioinformatics tool for elucidating small molecule signaling pathways that drive cells in a specific direction". *Cell Communication and Signaling* 11.1 (2013): 85.
39. Hecker N., *et al.* "SuperTarget goes quantitative: update on drug-target interactions". *Nucleic Acids Research* 40.D1 (2011): D1113-D1117.
40. Ning L., *et al.* "Current challenges in the bioinformatics of single cell genomics". *Frontiers in Oncology* 4 (2014): 7.
41. Kann MG. "Advances in translational bioinformatics: computational approaches for the hunting of disease genes". *Briefings in Bioinformatics* 11.1 (2009): 96-110.
42. Coassin S., *et al.* "Lost in the space of bioinformatic tools: a constantly updated survival guide for genetic epidemiology. The GenEpi Toolbox". *Atherosclerosis* 209.2 (2010): 321-335.
43. Kim P., *et al.* "TissGDB: tissue-specific gene database in cancer". *Nucleic Acids Research* 46.D1 (2017): D1031-D1038.

44. Cochrane G., *et al.* "Priorities for nucleotide trace, sequence and annotation data capture at the Ensembl Trace Archive and the EMBL Nucleotide Sequence Database". *Nucleic Acids Research* 36.1 (2007): D5-D12.
45. Huang DW., *et al.* "Bioinformatics enrichment tools: paths toward the comprehensive functional analysis of large gene lists". *Nucleic Acids Research* 37.1 (2008): 1-13.
46. Wood LD., *et al.* "The genomic landscapes of human breast and colorectal cancers". *Science* 318.5853 (2007): 1108-1113.
47. Zhao M., *et al.* "An evidence-based knowledgebase of pulmonary arterial hypertension to identify genes and pathways relevant to pathogenesis". *Molecular BioSystems* 10.4 (2014): 732-740.
48. Wang Q., *et al.* "VirusFinder: software for efficient and accurate detection of viruses and their integration sites in host genomes through next generation sequencing data". *PLoS one* 8.5 (2013): e64465.
49. Vandeweyer G., *et al.* "CNV-WebStore: online CNV analysis, storage and interpretation". *BMC Bioinformatics* 12.1 (2011): 4.
50. Jia P and Zhao Z. "VarWalker: personalized mutation network analysis of putative cancer genes from next-generation sequencing data". *PLoS Computational Biology* 10.2 (2014): e1003460.
51. Sacco LD., *et al.* "Bioinformatics tools and novel challenges in long non-coding RNAs (lncRNAs) functional analysis". *International Journal of Molecular Sciences* 13.1 (2011): 97-114.
52. Zheng S and Zhao Z. "GenRev: exploring functional relevance of genes in molecular networks". *Genomics* 99.3 (2012): 183-188.
53. Teo YM., *et al.* "GLAD: a system for developing and deploying large-scale bioinformatics grid". *Bioinformatics* 21.6 (2004): 794-802.
54. Mehboob-ur-Rahman TS., *et al.* "Bioinformatics: A Way Forward to Explore "Plant Omics". Bioinformatics-Updated Features and Applications (2016): 203.
55. Agapito G., *et al.* "Cloud4snp: distributed analysis of snp microarray data on the cloud". In Proceedings of the International Conference on Bioinformatics, Computational Biology and Biomedical Informatics. ACM (2013): 468.
56. Thorn CF., *et al.* "Pharmacogenomics and bioinformatics: PharmGKB". *Pharmacogenomics* 11.4 (2010): 501-505.
57. Lee F., *et al.* "Long-term follow-up of stages T2-T3 prostate cancer pretreated with androgen ablation therapy prior to radical prostatectomy". *Anticancer Research* 17.3A (1997): 1507-1510.
58. Davis AP., *et al.* "Comparative Toxicogenomics Database: a knowledgebase and discovery tool for chemical-gene-disease networks". *Nucleic Acids Research* 37.1 (2008): D786-D792.
59. Garnett MJ., *et al.* "Systematic identification of genomic markers of drug sensitivity in cancer cells". *Nature* 483.7391 (2012): 570-575.

Volume 2 Issue 3 March 2018

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